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Approach to the quantum mechanical many-body problem with strong two-particle interaction. II

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With 2 figures in the text

Introduction

In a previous paper [1] we have discussed variational methods for many-body systems with strong two-particle interaction with the use of wave functions built up from two-particle wave functions. General variational equations were derived, and simplified methods with parameter variation were discussed. One-dimensional systems were studied in some details, and for a system of bosons with Gaussian interaction explicit expressions were calculated with a simple choice of trial wave function.

As a preparation for the study of more realistic problems, we now make a more detailed analysis of a one-dimensional system of fermions with Gaussian interaction and with the corresponding simple trial wave function, in order to examine how the method works with strong short range interaction and to use the one-dimensional case as a starting point for the extension of the method to the three-dimensional case. Explicit calculations are made for a system of four three-dimensional fermions, and we close our work with a discussion of the application of the same method to the nuclear case.

When working with trial wave functions for many-body systems that are not built up of Slater-determinants of single particle wave functions, one usually has troubles to avoid complicated integrals. Even for the simplest trial wave functions our integrals will contain lots of terms, and in order to carry through the integrations without using approximate methods whose correctness is usually hard to estimate, it seems to be important to find integration methods that make use of all the symmetries in the expressions. Some details of our computations are given in an appendix.

System of one-dimensional fermions

We consider a system of n one-dimensional fermions with Gaussian interaction potential and a common oscillator potential. The Hamiltonian of the system can then be be written

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2} + \frac{m}{2}\omega^2\sum_{i=1}^{n} x_i^2 + \tfrac{1}{2} v_0 \sum_{i\neq j} \exp\{-\beta\,(x_i - x_j)^2\}. \qquad (1)$$

If we use the "Overlapping pair method" [1] and choose as two-particle wave function the function describing two particles with oscillator interaction and a common oscillator potential

$$f(x_1, x_2) = (x_1 - x_2) \exp\{-k_{\oplus}(x_1 + x_2)^2 - k_{\ominus}(x_1 - x_2)^2\},$$

then the trial wave function for the whole system is

$$\Psi(x_1 \dots x_n) = N \begin{vmatrix} H_0(x_1) \dots H_{n-1}(x_1) \\ \cdots\cdots\cdots \\ H_0(x_n) \dots H_{n-1}(x_n) \end{vmatrix} \times$$

$$\times \exp\{-(n-1)(k_{\oplus} + k_{\ominus}) \sum_{i=1}^{n} x_i^2 - (k_{\oplus} - k_{\ominus}) \sum_{i \neq j} x_i x_j\},$$

where $k_{\oplus}$ and $k_{\ominus}$ are the variational parameters that will be determined from the equation

$$\delta \langle H \rangle = 0.$$

The calculation of the explicit expression of $\langle H \rangle = E(k_{\oplus}, k_{\ominus})$ was made in (I) without much labour for the boson case, but in the fermion case the integrals will be complicated, due to the fact that the n-dimensional orthogonal transformation that transforms the exponentials to diagonal form must be applied to the polynomial A_n^2 of the degree $n(n-1)$, and this gives a great number of terms even for small n. For details of the integration, see the appendix. The expression for E as a function of the new dimensionless constants and parameters $\varkappa$, σ, γ and v, defined by

$$\left.\begin{array}{c} 2(n-1)(k_{\oplus} + k_{\ominus}) = \varkappa \dfrac{m\omega}{\hbar}, \qquad 2(k_{\oplus} - k_{\ominus}) = \nu \dfrac{m\omega}{\hbar}, \qquad v_0 = \tfrac{1}{2} v \hbar \omega, \\ \beta = \gamma \dfrac{m\omega}{\hbar} \quad \text{and} \quad \varkappa - \nu = \sigma, \end{array}\right\} \qquad (2)$$

is

$$E(\varkappa, \sigma) = \tfrac{1}{2}\hbar\omega \left[\frac{n}{2}\varkappa + \tfrac{1}{2}n(n-1)\sigma + \frac{1}{2n\varkappa - 2(n-1)\sigma} + \frac{n^2 - 1}{2\sigma} + \right.$$

$$\left. + \frac{n(n-1)}{2} v \sqrt{\frac{\sigma}{\sigma + \gamma}} P_n\left(\frac{\sigma}{\sigma + \gamma}\right)\right],$$

where P_n is a polynomial. In the appendix the coefficients are given for $n = 2$, 3 and 4.

This expression for the total energy of the system will now be minimized with respect to the parameters $\varkappa$ and σ.

$$\frac{\partial E}{\partial \varkappa} = 0 \quad \text{gives} \quad n\varkappa - (n-1)\sigma = 1 \quad \text{or} \quad \varkappa + (n-1)\nu = 1.$$

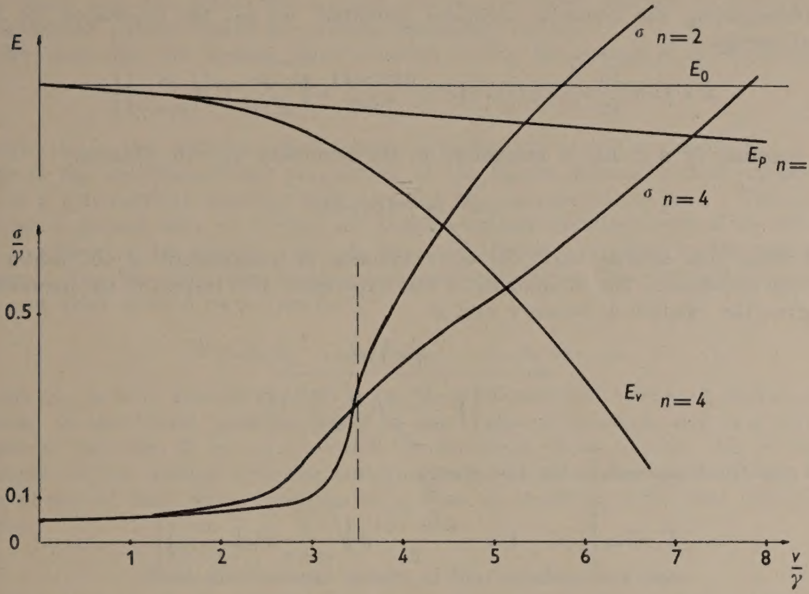

Fig. 1. The dependence of structure-determining parameter σ on the strength of the interaction v, is given for linear systems with two and four particles. If the figure is extended to higher v-values, the curves intersect again for $v/\gamma \approx 15$. The energies of the system E_v and E_p obtained by the variational method and by a first order perturbation calculation, are also given as a function of v for the four-particle system. The line of short dashes indicates the smallest strength of the interaction $v_{\min}$, for which bound two-particle states exists. A comparison of the two energy calculations shows that the first order perturbation can be good for an interaction strength up to $\frac{1}{2}\, v_{\min}$, but in the vicinity of $v_{\min}$, it seems to be very bad. The interaction range is chosen rather short, $\gamma = 20$.

The interpretation of this is that the center of gravity motion corresponds to an oscillator motion with the frequency ω. We have then

$$E(\sigma) = \tfrac{1}{2}\hbar\omega\left[1 + \frac{n^2-1}{2}\left(\sigma + \frac{1}{\sigma}\right) + \frac{n(n-1)}{2}\, v \sqrt{\frac{\sigma}{\sigma+\gamma}}\, P_n\left(\frac{\sigma}{\sigma+\gamma}\right)\right].$$

$\partial E/\partial \sigma = 0$ gives the relation between v and σ

$$v = \frac{n+1}{n}\,\frac{1/\sigma^2 - 1}{\dfrac{\partial}{\partial\sigma}\left[\sqrt{\dfrac{\sigma}{\sigma+\gamma}}\, P_n\left(\dfrac{\sigma}{\sigma+\gamma}\right)\right]}.$$

Without interaction between the particles ($v = 0$) we have $\sigma = 1$, and the wave function describes, as required, a system of n independent Fermi-oscillators with the frequency ω.

The dependence of σ on v is given in Fig. 1. σ appears here as the single structure-describing parameter, and its deviation from 1 determines the deviation from independent particle state.

Disregarding the common oscillator potential, we get the expression for the total energy

$$E=\tfrac{1}{2}\hbar\,\omega\left[\frac{n}{2}\varkappa+\tfrac{1}{2}n\,(n-1)\,\sigma+\frac{n\,(n-1)}{2}v\sqrt{\frac{\sigma}{\sigma+\gamma}}\,P_n\left(\frac{\sigma}{\sigma+\gamma}\right)\right].$$

As function of $\varkappa$ it has a minimum on the boundary $k_{\ominus}=0$, that is

$$n\varkappa-(n-1)\,\sigma=0,$$

and from this follows that the wave function is independent of the center of gravity coordinate. The minimizing of this expression with respect to the parameter σ gives the relation between v and σ

$$v=\frac{(n+1)/n}{\dfrac{\partial}{\partial\sigma}\left[\sqrt{\dfrac{\sigma}{\sigma+\gamma}}\,P_n\left(\dfrac{\sigma}{\sigma+\gamma}\right)\right]}$$

and the final expression for the energy

$$E=\hbar\,\omega\left[\tfrac{1}{2}(n^2-1)\,\sigma-\frac{n\,(n-1)}{2}v\sqrt{\frac{\sigma}{\sigma+\gamma}}\,P_n\left(\frac{\sigma}{\sigma+\gamma}\right)\right].$$

The least value of v for which solutions of σ exist, can be interpreted as the weakest interaction for which bound states exist.

Ordinary perturbation theory, with the two-particle interaction term as perturbation term, gives to the first order

$$E-E_0=\tfrac{1}{2}\hbar\,\omega\,v\sqrt{\frac{1}{1+\gamma}}\,P_n\left(\frac{1}{1+\gamma}\right).$$

This energy expression is compared with the corresponding expression obtained from the variational treatment in Fig. 1.

Three-dimensional system of Fermi-particles

In the three-dimensional case it seems to be hard to find any two-particle trial wave function that gives a simple parameter wave function for the whole system with the required property of giving the correct wave function for a system of free particles for certain values of the parameters, if we use the "overlapping pair model" for the building up of the system wave function. With the "disjoint pair model" (see part I) it is certainly possible to construct two-particle wave functions that give such a system wave function. This wave function, however, properly antisymmetrised, consists of a sum of terms each lacking symmetry between the particles, and is therefore hard to handle. For the following discussion of three-dimensional systems we therefore choose to give up our starting-point that the wave function for the system will be constructed from two-particle wave functions, and instead choose the system wave function in direct analogy with the linear case but retain the requirement on the wave function to describe an independent particle state for certain parameter values.

We note that our system wave function in the linear case is of the form

$$\Psi = A_n(x_1, \ldots, x_n)\, S_n(x_1, \ldots, x_n, p_1, p_2, \ldots),$$

where A_n is the antisymmetrical basic invariant [2] in the variables $x_1, \ldots, x_n$. This is the antisymmetrical polynomial of the lowest degree in these variables. S_n is a symmetrical function that contains the parameters $p_1, p_2, \ldots$. This is of course a general way of writing an antisymmetrical function, even if we restrict all functions to be regular. (For A_n has only the zeros required by the antisymmetry.) For the three-dimensional case we now choose the corresponding form for our trial system wave function

$$\Psi = A_n(r_1, \ldots, r_n)\, S_n(r_1, \ldots, r_n, p_1, p_2, \ldots),$$

where A_n is now antisymmetrical in the three-dimensional vectors r_i and a polynomial of the lowest possible degree in the vector-components, and S_n is a symmetrical function. If we now restrict the functions to be regular, this is not a general way of writing a regular antisymmetrical function, but we have restricted our choice of trial wave functions to a class of functions with some prescribed zeros.

Three-dimensional system of four spinless fermions

For four particles $A_4(r)$ is uniquely determined and rotational invariant. If we now choose as a simple example a system with central Gaussian interaction between the particles and a common isotropic oscillator potential, we must assume the ground state to be an S-state and must then choose S_4 to be rotational invariant, too.

As a trial wave function we now use

$$\Psi = N\, A_4(r)\, S_4$$

and in analogy with the linear case we choose

$$S_4 = \exp\{-b(r)\},$$

where

$$b(r) = \sum_{i \neq j} [k_{\oplus}(r_i + r_j)^2 + k_{\ominus}(r_i - r_j)^2] = \sum_{\eta = x,\, y,\, z} \left[\varkappa \sum_{i=1}^{n} \eta_i^2 + \nu \sum_{1 \leq i < j \leq n} \eta_i \eta_j \right]; \tag{3}$$

$\varkappa$ and σ are given by (2).

The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{n} \Delta_i + \frac{m}{2} \omega^2 \sum_{i=1}^{n} r_i^2 + \tfrac{1}{2} v_0 \sum_{i \neq j} \exp\{-\beta (r_i - r_j)^2\}. \tag{4}$$

The calculation of the expectation value of the total energy is now very easy (see appendix), and we get the following expression for E in the same parameters as in the linear case:

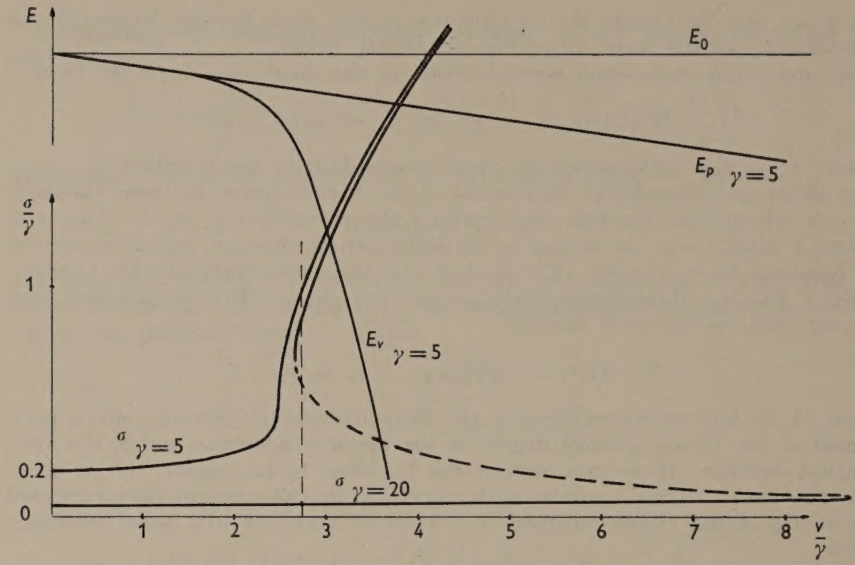

Fig. 2. The dependence of the parameter σ and the energy E on v is given for the three-dimensional four-particle system with two different ranges of the interaction, $\gamma = 5$ and 20. When the interaction is of short range, $\gamma > 5$, there is a discontinuous change in σ when v passes a value slightly higher than $v_{\min}$. See text to Fig. 1.

$$E(\varkappa, \sigma) = \tfrac{1}{2}\hbar\omega\left[3(2\varkappa+\sigma) - 12v\left(\frac{\sigma}{\sigma+\gamma}\right)^{5/2} + \tfrac{1}{2}\left(\frac{15}{\sigma} + \frac{3}{4\varkappa - 3\sigma}\right)\right].$$

The minimizing of this expression with respect to $\varkappa$ gives the relation $4\varkappa - 3\sigma = 1$, which means that the center of gravity of the system moves as an oscillator with the frequency ω. We have then

$$E(\sigma) = \tfrac{1}{2}h\omega\left[3 + \tfrac{15}{2}\left(\sigma + \frac{1}{\sigma}\right) - 12v\left(\frac{\sigma}{\sigma+\gamma}\right)^{5/2}\right],$$

and the second minimizing equation, $\partial E/\partial\sigma = 0$, gives the relation between v and σ

$$v = \frac{1}{4}\,\frac{(1-1/\sigma^2)(\sigma+\gamma)^3}{\sigma\gamma\sqrt{\sigma/(\sigma+\gamma)}}.$$

Neglecting the common potential, we get

$$v = \frac{1}{4}\,\frac{(\sigma+\gamma)^3}{\sigma\gamma\sqrt{\sigma/(\sigma+\gamma)}},$$

and this function has a minimum for $\sigma/\gamma = \tfrac{5}{2}$, which may again be interpreted as the weakest potential for which bound states exist.

$$v_{\min} = 2.72\,\gamma.$$

The dependence of E and σ on v is given in Fig. 2.

Particles with spin

The straight forward extension of the method to particles with spin is to introduce the ordinary spin-coordinate σ with the possible values $+1$ and -1, and to define the antisymmetrical basic invariant as the polynomial in the variables x_i, y_i, z_i, and σ_i, $i=1, \ldots, n$, that is antisymmetrical in index exchange and is of the lowest possible degree in the Cartesian coordinates.

For a system with spin independent Hamiltonian we then make the corresponding assumption for the wave function

$$\Psi(r_1, \ldots, r_n, \sigma_1, \ldots, \sigma_n) = A_n(r, \sigma)\, S_n(r_1, \ldots, r_n, p_1, p_2, \ldots),$$

where S_n is independent of the spin coordinate. For certain values of n, $A_n(r, \sigma)$ is not uniquely determined, and then the ground state level is degenerated. A weak spin-dependent interaction will usually split this degeneracy, but we can assume that the main influence of the spin-dependent term on the ground state wave function is on the choice of the right A_n, and that S_n will be the same function for all these degenerated states, and that the parameter values can be determined from the Hamiltonian without the spin-dependent term. For strong spin-dependent forces it is certainly not possible to get a useful trial wave function in this manner, but a different A_n must be chosen, and S_n may perhaps depend on the spin coordinate.

Suggestion for the nuclear problem

To follow the same line in the construction of a trial wave function for the atomic nucleus we construct in the same way the basic invariant $A_n(r, \sigma, \tau)$ and try to find a suitable S_n that depends on a number of parameters for the wave function

$$\Psi(r, \sigma, \tau) = A_n(r, \sigma, \tau)\, S_n(r, p_1, p_2, \ldots).$$

It is now tempting to assume that S_n is a function that varies in a uniform manner with the particle number and contains the main properties of nuclear matter (including also the size of the nuclei), and that A_n that varies irregularly with n, describes the main part of the individual properties in the nuclear table. However, even if the nuclear forces are charge independent, there is certainly a strong spin dependence, and the coulomb force will have a strong influence on the wave function; so it is only for light nuclei that one can use the basic invariants A_n with any hope of success. If we retain our requirement of S_n to be regular and of the wave function to describe an independent particle state for certain parameter values, we are forced to use other antisymmetrical polynomials than the basic invariants for heavier nuclei. Possibly one can construct these polynomials of higher degree than the lowest with the guidance of shell model calculations. If one uses such a nuclear wave function with a uniformly varying S_n, it would be of interest to examine if the main results of the shell model calculations remain with an S-function which departs from one describing an independent particle state.

Comparison with the Jastrow method

Jastrow [3] has proposed a variational approach to the quantum mechanical many-body problem, with a trial wave function for a fermion system of the form

$$\Psi = \prod_{i<j} f(r_{ij})\, \Psi_s,$$

where Ψ_s is a Slater-determinant of single particle orbitals, and $f(r_{ij})$ is a correlation function depending on the distance betweeen the particles i and j. $f(r_{ij})$ contains also variational parameters. Several authors [4, 5] have used this form of trial wave functions for the study of the so-called nuclear matter. They use for the calculation of their integrals the so-called cluster development method, i.e. an expansion of the two-particle density function in terms containing integrals over an increasing number of f-functions.

We can write our trial wave function for the linear system in the following form

$$\Psi = \exp\left\{(\sigma - 1) \sum_1^n x_i^2 + \nu \sum_{1 \le i < j \le n} x_i x_j\right\} \times \exp\left\{\sum_1^n x_i^2\right\} A_n,$$

and this wave function corresponds to a Jastrow wave function with

$$f(x_{ij}) = \exp\left\{(\sigma - 1) \sum_1^n x_i^2 + \nu \sum_{1 \le i < j \le n} x_i x_j\right\},$$

and with the variational parameters σ and ν.

APPENDIX

Here are given some details from the integrations of the expressions for the expectation values of the energies.

The linear case

The integral for the energy-expectation-value is

$$E = N^2 \int_{-\infty}^{\infty} A_n(x) \exp\left\{-\tfrac{1}{2} b(x)\right\} H A_n(x) \exp\left\{-\tfrac{1}{2} b(x)\right\} dx_1 \dots dx_n,$$

where
$$\frac{1}{N^2} = \int_{-\infty}^{\infty} A_n^2 \exp\left\{-b(x)\right\} dx_1 \dots dx_n,$$

$$A_n(x) = \prod_{1 \le i < j \le n} (x_i - x_j) = \begin{vmatrix} 1 & x_1 & x_1^2 & x_1^3 \dots x_1^{n-1} \\ \cdot & \cdot & \cdot & \cdot \\ 1 & x_n & x_n^2 & x_n^3 \dots x_n^{n-1} \end{vmatrix}$$

and the function in the exponent

$$b(x) = \varkappa \sum_i x_i^2 + \nu \sum_{i<j} x_i x_j \quad \left(x \text{ is } \frac{\mathrm{m}}{\hbar\omega} \times \text{length}\right).$$

The Hamiltonian H of the system is given by (1). The interaction term in the Hamiltonian gives an additional term, $\beta \sum_{i<j} (x_i - x_j)^2$, in the exponent, and we have to solve integrals consisting of polynomials multiplied by exponential functions of the argument

$$b'(x, \beta) = \varkappa \sum_i x_i^2 + \sum_{i<j} x_i x_j + \beta (x_1 - x_2)^2.$$

This quadratic form is now "diagonalised" by the solution of the corresponding secular equation. The roots of this equation are simply obtained by elementary determinantal transformations. One gets the following expression for the quadratic form in the new variables

$$b'(x, \beta) = (\varkappa + (n-1)\nu)\,\xi_1^2 + (\varkappa - \nu + 2\beta)\,\xi_2^2 + \sum_{i=3}^{n} (\varkappa - \nu)\,\xi_i^2.$$

The direction of the new coordinate axis in the n-dimensional space can be represented by the vectors $\bar{e}_1, \ldots, \bar{e}_n$, where $\bar{e}_1 = (1, 1, \ldots, 1)$ and the other vectors are orthogonal. This is sufficient to "diagonalise" $b(x)$, but for $b'(x, \beta)$ one must choose one of the vectors to have the direction $(1, -1, 0, \ldots, 0)$. A_n can be written as the product of the $n(n-1)/2$ planes

$$\bar{n}_{ij} \cdot \bar{r} = 0$$

with the normal vectors $\bar{n}_{ij} = (0, \ldots, 0, 1, 0, \ldots, 0, 1, 0, \ldots, 0)$, where 1 and -1 stand on the coordinate places i and j. All the planes intersect in the line $(1, 1, \ldots, 1)$.

We have then

$$A_n = \prod_{i<j} (\bar{n}_{ij} \cdot \bar{r}).$$

We now get the expression for A_n in the new coordinates, if we express the normal vectors in their components in the new coordinate system with the direction vectors $\bar{e}_1, \ldots, \bar{e}_n$.

When $\bar{e}_1$ and $\bar{e}_2$ are fixed, one can choose the other direction vectors in different manners. A general and simple way to construct them is

$$\begin{array}{ll} e_1 = (1, 1, \ldots, 1) & e_4 = (1, 1, 1, -3, 0, \ldots, 0) \\ e_2 = (1, -1, 0, \ldots, 0) & e_5 = (1, 1, 1, 1, -4, 0, \ldots, 0) \\ e_3 = (1, 1, -2, 0, \ldots, 0) & \text{a.s.o.} \end{array}$$

With these new axis directions we get the expression for A_n in the new coordinates

$$A_n = \prod_{i<j} a_{ij},$$

where

$$a_{ij} = -(i-1)\,\xi_i + \sum_{k=i+1}^{j-1} \xi_k + j\,\xi_j.$$

For certain n-values it is possible to choose the axis directions in a more symmetric way. For $n = 4$ we have used for our computations the axis directions

$$\begin{array}{ll} \bar{e}_1 = (1, 1, 1, 1), & \bar{e}_2 = (1, -1, 0, 0), \\ \bar{e}_3 = (0, 0, 1, -1), & \bar{e}_4 = (1, 1, -1, -1). \end{array}$$

If $n = 2^m$, where m is an integer, it is possible to construct the vectors in a corresponding manner.

The integrations now give the energy expressions

$$\langle T \rangle = \frac{\hbar^2}{2m} \left[\frac{n}{2} \varkappa + (\varkappa - \nu) \left\{ \frac{n-1}{2} + f_1(n) + 2 f_2(n) \right\} \right]$$

and

$$\langle V_{\text{pot.}} \rangle = \frac{m}{4} \omega^2 \left[\frac{1}{\varkappa + (n-1)\nu} + \frac{2 f_1(n)}{(\varkappa - \nu)} \right],$$

where

$$f_1(n) = \frac{(\varkappa - \nu)}{N^2} \int_{-\infty}^{\infty} A_n^2 \sum_{i=2}^{n} \xi_i^2 \exp\{-b(\xi)\} \, d\xi_1 \ldots d\xi_n$$

and

$$f_2(n) = \frac{1}{N^2} \int_{-\infty}^{\infty} A_n \sum_{i=2}^{n} \left(\xi_i \frac{\partial}{\partial \xi_i} A_n \right) \exp\{-b(\xi)\} \, d\xi_1 \ldots d\xi_n.$$

It is not necessary to carry out the integrals for f_1 and f_2, when we observe that they are independent on $\varkappa$ and σ, and that with $\nu = 1$ and $\varkappa = m\omega/\hbar$ the wave function describes noninteracting Fermi oscillators, where we have $\langle T \rangle = \langle V_{\text{pot.}} \rangle = \frac{1}{4} n^2 \hbar \omega$. We then get

$$\langle T \rangle = \frac{\hbar^2}{2m} \left[\frac{n}{2} + \frac{1}{2} n (n-1)(\varkappa - \nu) \right],$$

$$\langle V_{\text{pot.}} \rangle = \frac{m}{4} \omega \frac{1}{\varkappa + (n-1)\nu} + \frac{n^2 - 1}{(\varkappa - \nu)}.$$

The integral for the expectation value of the interaction energy gives

$$\langle V_{\text{int.}} \rangle = v_0 \frac{n(n-1)}{2} \sqrt{\frac{\varkappa - \nu}{\varkappa - \nu + \beta}} \, P_n \left(\frac{\varkappa - \nu}{\varkappa - \nu + \beta} \right),$$

where P_n is a polynomial. A general formula for the coefficients of P_n must be very complicated, and we have only calculated its coefficients for n up to four.

If
$$P_n(x) = \sum_{\nu=0}^{2n-4} a_\nu^n x^\nu,$$

we have for the coefficients a_ν^n

ν \ n	2	3	4
0	1	1.125	1.3032 ...
1		−0.75	−1.9310 ...
2		0.625	2.4976 ...
3			−2.4355 ...
4			1.5657 ...

The three-dimensional case with four fermions

The integral for the expectation value of the energy is here

$$E=\frac{1}{N^2}\int_{-\infty}^{\infty} A_4(r)\exp\{-b(r)\}\,H\,A_4(r)\exp\{-b(r)\}\,d^3r_1\,d^3r_2\,d^3r_3\,d^3r_4,$$

where
$$A_4(r)=\begin{vmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{vmatrix}$$

and $b(r)$ is given by (3) with $n=4$. H is given by (4). $A_4(r)$ can now be written

$$A_4(r)=c\sum P_{x,y,z}(-1)^p(\bar{n}_1\cdot\bar{x})(\bar{n}_2\cdot\bar{y})(\bar{n}_3\cdot\bar{z})$$

$$=c\sum P_{1,2,3}\,(-1)^p(\bar{n}_1\cdot\bar{x})(\bar{n}_2\cdot\bar{y})(\bar{n}_3\cdot\bar{z}).$$

The sums are taken over all permutations P, and p is the number of inversions in the permutation. The bar here means four-dimensional vectors, and $\bar{n}_1$, $\bar{n}_2$, $\bar{n}_3$ and the axis (1, 1, 1, 1) are orthogonal. (The vectors $\bar{n}$ ought here not to be mutually orthogonal but linearly independent.) These directions are, properly chosen, also principal axis of the quadratic forms in the exponent, and we choose them as our new coordinate axis. We then get the simple expression for $A_4(r)$

$$A_4(r)=\sum P_{x,y,z}(-1)^p x_2 y_3 x_4=\sum P_{2,3,4}(-1)^p x_2 y_3 z_4,$$

where the numbers now mean vector components in our new four-dimensional coordinate system.

Because of the simple invariance properties of the Hamiltonian for this coordinate transformation, the integrals are very simple, and we get without much labour

$$\langle T\rangle=\frac{9\hbar^2}{2m}\left(\varkappa-\frac{\nu}{3}\right),$$

$$\langle V_{\text{pot.}}\rangle=\frac{m\omega^2}{4}\left(\frac{15}{\varkappa-\nu}+\frac{3}{\varkappa+3\nu}\right),$$

$$\langle V_{\text{int.}}\rangle=6\left(\frac{\varkappa-\nu}{\varkappa-\nu+\beta}\right)^{5/2}.$$

The present investigation was carried out at the Institute of Theoretical Physics in Stockholm, and I wish to thank Professor O. Klein, Director of the Institute, for his kind interest in this work.

Institute of Theoretical Physics, Stockholm, November 1958.

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